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WarpX: Delivering Unprecedented Particle-in-Cell Simulation Capability

C. N. Meissner

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WarpX: Delivering Unprecedented Particle-in-Cell Simulation Capability

Since 1939, more than 30 percent of all Nobel prizes in physics and four of the past 14 prizes in chemistry have been awarded for work with particle accelerators. These tools are now used to treat cancer and produce medical supplies, support research in applied fields such as pharmaceuticals, create microcircuits, and sterilize food—and the applications list continues to grow. However, the size of the facilities needed to house these machines—which are often dozens of kilometers long—has limited their future potential. Thus, researchers are motivated to create novel particle accelerator designs that provide new imaging capability but have a much smaller footprint. The Exascale Computing Project's WarpX application captures the full complexity of the acceleration processes within plasma-based design, supporting the rapid and cost-efficient development of tens of thousands of new particle accelerators for various applications from improving human health to nuclear fusion reactors.

A Winning Combination

The development of plasma-based particle accelerators depends critically on high-performance, high-fidelity modeling to capture relevant processes as they develop over a large range of space and timescales and to study various phenomena—including injection, emittance transport, beam loading, tailoring of the plasma channel, and tolerance to non-ideal effects. However, simulations of plasma accelerators are computationally intensive as they need to resolve the evolution of a driver (laser or particle beam) and an accelerated beam into a structure that is orders of magnitude longer and wider than the accelerated beam. WarpX combines the AMReX adaptive mesh refinement framework with novel computational techniques that were pioneered in the predecessor particle-in-cell (PIC) code Warp to optimize the code for parallel computing on exascale systems and produce faster, larger, and higher fidelity 3D models of laser–matter interactions.

The Future Looks Bright

As part of ECP, the WarpX team incorporated and improved the most advanced algorithms, including the optimal Lorentz boosted frame approach, scalable spectral electromagnetic solvers, and mitigation methods for the numerical Cherenkov instability, and developed new algorithms to enhance code performance. To ensure speed and scalability, WarpX takes advantage of performance-portable, parallel C++ primitives for mesh-refined, particle-mesh routines in AMReX, as well as dynamic load-balancing the computational work. It further integrates modern linear algebra routines from SLATE for advanced geometries, advanced I/O routines from ADIOS, and *in situ* visualization from Ascent to compute and analyze plasma accelerator modeling challenges at scale.

Since the team began working on the ECP project in 2016, WarpX now runs 500 times faster than the previous version of the code. WarpX was the first application project in ECP to run on the full scale of Frontier. In 2022, the WarpX team won the coveted Gordon Bell Prize from the Association for Computing Machinery for successfully implementing and deploying WarpX to deliver significantly advanced particle-in-cell simulations of kinetic plasma optimized on 4 of the 10 fastest supercomputers in the world. Going forward, WarpX simulations will increase the pace of accelerator development and will greatly reduce the costs associated with planning, constructing, and iterating on plasma-based collider designs. The team is also expanding on WarpX's potential applications—building an ecosystem that can be used for plasma accelerator modeling but also conventional accelerators as well as laboratory and space plasma research, fusion energy, and more.

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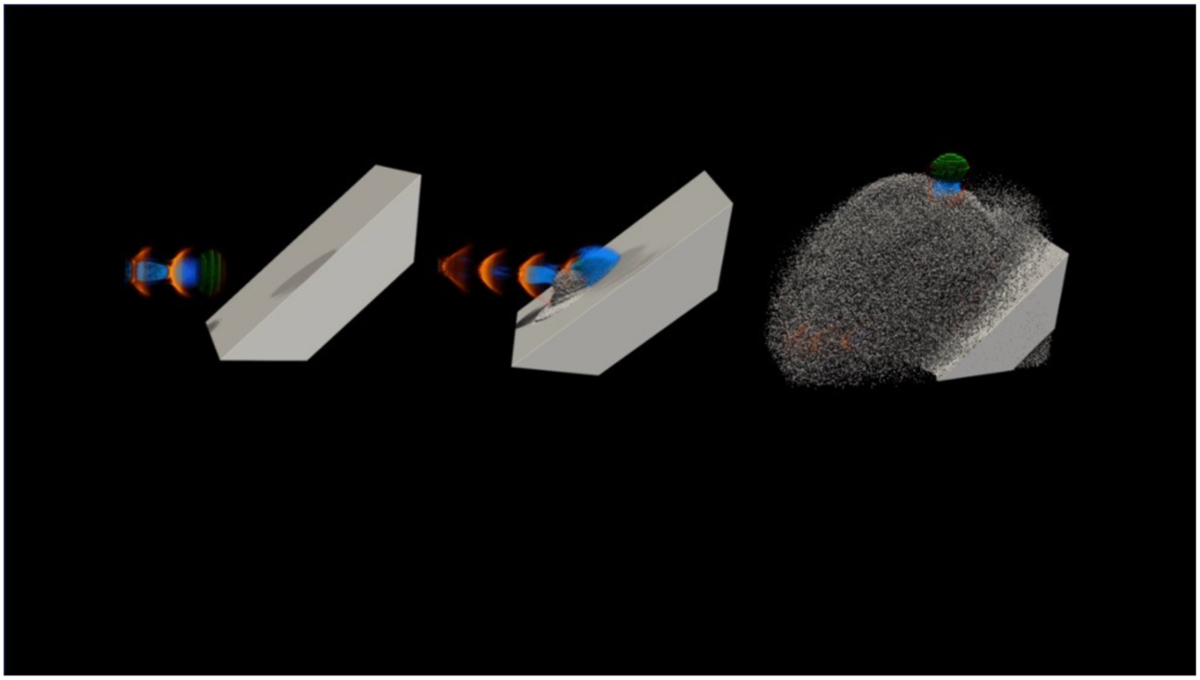

Using the Frontier supercomputer, the WarpX team produced a 3D simulation at scale of their own novel concept: a combined plasma particle injector and accelerator, which focuses a high-power femtosecond (1 quadrillionth of a second) laser onto a hybrid solid/gas target. The simulation's predictions were later validated by a proof-of-concept experiment performed on the Salle Jaune laser at Laboratoire d'Optique Appliquée in France by Adrien Leblanc and other CEA collaborators. Image credit: Dave Pugmire/ORNL